

Exact solution, scaling behaviour and quantum dynamics of a model of an atom-molecule Bose-Einstein condensate

Huan-Qiang Zhou*, Jon Links and Ross H. McKenzie

Centre for Mathematical Physics, The University of Queensland, 4072, Australia

We study the exact solution for a two-mode model describing coherent coupling between atomic and molecular Bose-Einstein condensates (BEC), in the context of the Bethe ansatz. By combining an asymptotic and numerical analysis, we identify the scaling behaviour of the model and determine the zero temperature expectation value for the coherence and average atomic occupation. The threshold coupling for production of the molecular BEC is identified as the point at which the energy gap is minimum. Our numerical results indicate a parity effect for the energy gap between ground and first excited state depending on whether the total atomic number is odd or even. The numerical calculations for the quantum dynamics reveals a smooth transition from the atomic to the molecular BEC.

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After the experimental realization of a Bose-Einstein condensate (BEC) in dilute alkali gases [1], many physicists started to consider the possibility of producing a molecular Bose-Einstein condensate from photoassociation and/or the Feshbach resonance of an atomic Bose-Einstein condensate [2,3]. As discussed by Zoller [4], this tantalizing problem is now coming toward resolution. Donley *et al.* [5] recently reported the creation of a BEC of coherent superpositions of atomic and molecular ^{85}Rb states. This achievement is significant in that the entangled state is comprised of two chemically distinct components.

In anticipation of this result, this novel area has attracted considerable attention from theoretical physicists [6–14]. Drummond *et al.* [6,9] emphasized the finite-dimensionality of the system and the importance of quantum fluctuation. Javanainen *et al.* [7] systematically analysed the efficiency of photoassociation of an atomic condensate into its molecular counterpart. In Refs. [7–9], large-amplitude coherent oscillations between an atomic BEC and a molecular BEC were predicted through the use of the Gross-Pitaevski (GP) mean-field theory (MFT). Others have gone beyond the GP-MFT [13,14]. Vardi *et al.* [12] suggested that the large-amplitude atom-molecule coherent oscillations are damped by the rapid growth of fluctuations near the dynamically unstable molecular mode, which contradicts the MFT predictions. This has caused some disagreement regarding the atom-molecule conversion and the nature of coherence [5]. In order to clarify the controversies raised by these investigations, it is highly desirable to extract some rigorous and analytical results.

The aim of this Letter is to show that a model Hamiltonian to describe coherent coupling between atomic and molecular BEC's described by single modes is exactly solvable in the context of the algebraic Bethe ansatz [15]. This makes it feasible to apply techniques well-established in the mathematical physics literature to

study the physics behind this new phenomenon. The Bethe ansatz equations are analysed and solved asymptotically in the limits of the stable molecular regime and the stable atomic regime. Numerical solutions are also obtained for the crossover regime. We identify a scaling invariance for the model and show that the exact solution predicts a smooth transition from a quasi-periodic and stable regime to a coherent, large-amplitude, non-periodic oscillating regime. For finite particle number there are no stationary points in contrast to the prediction by Vardi *et al.* using a linearization scheme [12]. Instead, the onset of strong entanglement as the detuning is decreased is identified as the point at which the energy gap to the first excited state takes the minimum value.

The Hamiltonian takes the form

$$H = \frac{\delta}{2} \hat{a}^\dagger \hat{a} + \frac{\Omega}{2} (\hat{a}^\dagger \hat{a}^\dagger \hat{b} + \hat{b}^\dagger \hat{a} \hat{a}), \quad (1)$$

where \hat{a}^\dagger and \hat{b}^\dagger denote the creation operators for atomic and molecular modes, respectively, Ω is a measure of the strength of the matrix element for creation and destruction of molecules, and δ is the molecular binding energy in the absence of coupling. A similar Hamiltonian was first used to describe optical second harmonic generation [16] and (with additional damping terms) photon squeezing experiments in a two-mode interferometer [17]. It was recently investigated by Vardi *et al.* [12] as a model for atom-molecule BEC's. Note that the total atom number operator $\hat{N} = \hat{n}_a + 2\hat{n}_b$, where $\hat{n}_a = \hat{a}^\dagger \hat{a}$, $\hat{n}_b = \hat{b}^\dagger \hat{b}$, provides a good quantum number since $[H, \hat{N}] = 0$.

Bethe ansatz solution. Following the procedure of the algebraic Bethe ansatz [15], we have derived the Bethe ansatz equations (BAE) which solve the model (1). For given quantum number M the BAE for the spectral parameters $\{v_i\}$ read

$$\frac{\delta}{\Omega} - v_i + \frac{2k}{v_i} = 2 \sum_{j \neq i}^M \frac{1}{v_j - v_i}. \quad (2)$$

Above, k is a discrete variable which takes values $1/4$ or $3/4$, dependent on whether the total number of particles is even or odd respectively. More specifically we have $N = 2M + 2(k - 1/4)$. For each M there are $2M + 1$ families of solutions $\{v_i\}$ to (2). For a given solution, the corresponding energy eigenvalue is

$$E = \delta M + \delta(k - 1/4) - \Omega \sum_{i=1}^M v_i. \quad (3)$$

Although we will not derive the BAE here, we remark that the model is obtained through a product of the Lax operators for the $su(1, 1)$ algebra [18,19] and the Heisenberg algebra [20] in the quasi-classical limit. The construction is similar to that used in the solution of the generalized Tavis-Cummings model from quantum optics [18,19]. The eigenstates are also obtained through this procedure. Consider the following class of states

$$|v_1, \dots, v_M\rangle = \prod_{i=1}^M C(v_i) |\Psi\rangle \quad (4)$$

where $C(v) = (v\hat{b}^\dagger - \hat{a}^\dagger\hat{a}^\dagger/2)$, $|\Psi\rangle = |0\rangle$ for $k = 1/4$ and $|\Psi\rangle = \hat{a}^\dagger|0\rangle$ for $k = 3/4$. In the case when the set of parameters $\{v_i\}$ satisfy the BAE then (4) are precisely the eigenstates of the Hamiltonian.

Asymptotic analysis. In the limit of large $|\delta/\Omega|$ we can perform an asymptotic analysis of the Bethe ansatz equations to determine the asymptotic form of the energy spectrum. We choose the following ansatz for the Bethe roots

$$\begin{aligned} v_i &\approx \mu_i \Omega / \delta & i &\leq m, \\ v_i &\approx \delta / \Omega + \epsilon_i + \mu_i \Omega / \delta & i &> m. \end{aligned}$$

Substituting into the BAE and solving for ϵ_i, μ_i leads to the following asymptotic result for the energy spectrum (cf. [21])

$$\begin{aligned} E_m &\approx \delta(m + k - 1/4) \\ &\quad + \Omega^2(3m^2 - m + 4km - 2kM - 2mM)/\delta. \end{aligned}$$

This result can be confirmed by second-order perturbation theory. The level spacings $\Delta_m = E_m - E_{m-1}$ are found to be

$$\Delta_m \approx \delta - 2\Omega^2(M + 2 - 3m - 2k)/\delta.$$

We let \mathcal{E} denote the ground state energy and Δ the gap to the first excited state. Employing the Hellmann-Feynman theorem we can determine the asymptotic form of the following zero temperature correlations

$$\langle \hat{n}_a \rangle = 2 \frac{\partial \mathcal{E}}{\partial \delta}, \quad \theta = 2 \frac{\partial \mathcal{E}}{\partial \Omega}$$

where $\theta \equiv -\langle \hat{a}^\dagger \hat{a}^\dagger \hat{b} + \hat{b}^\dagger \hat{a} \hat{a} \rangle$ is the *coherence correlator*. We then have for large $\delta/(\Omega N^{1/2}) > 0$

$$\frac{\Delta}{\Omega N^{1/2}} \approx \frac{\delta}{\Omega N^{1/2}} - \frac{\Omega N^{1/2}}{\delta}, \quad \frac{\langle n_a \rangle}{N} \approx 0, \quad \frac{\theta}{N^{3/2}} \approx 0$$

while for large $\delta/(\Omega N^{1/2}) < 0$

$$\frac{\Delta}{\Omega N^{1/2}} \approx -\frac{\delta}{\Omega N^{1/2}} - 2 \frac{\Omega N^{1/2}}{\delta}, \quad \frac{\langle n_a \rangle}{N} \approx 1 - \frac{\Omega^2 N}{2\delta^2},$$

$$\frac{\theta}{N^{3/2}} \approx -\frac{\Omega N^{1/2}}{\delta}.$$

The above results suggest that the model has scale invariance with respect to the single variable $\Omega N^{1/2}/\delta$. They also suggest that the scaled gap $\Delta/(\Omega N^{1/2})$ will have a minimum at some positive value of $\Omega N^{1/2}/\delta$ of the order of unity. However, as the above is an asymptotic result, we need to undertake a numerical analysis to obtain a more precise picture for the region of small $|\delta/(\Omega N^{1/2})|$, and to establish that the scaling is also valid in this region.

Numerical analysis. There is a convenient method to determine the energy spectrum without solving the BAE. This is achieved by resorting to the functional Bethe ansatz [22]. Let us introduce the polynomial function whose zeros are the roots of the BAE; viz.

$$G(u) = \prod_{i=1}^M (1 - u/v_i).$$

It can be shown from the BAE that G satisfies the differential equation

$$uG'' - (u^2 - \delta u - 2k)G' + (Mu - E + \delta(k - 1/4))G = 0$$

subject to the initial conditions $G(0) = 1$, $G'(0) = E - \delta(k - 1/4)/2k$. By setting $G(u) = \sum_{n=0}^M g_n u^n$ the recurrence relation

$$g_{n+1} = \frac{E - \delta(n + k - 1/4)}{\Omega(n+1)(n+2k)} g_n + \frac{n - M - 1}{(n+1)(n+2k)} g_{n-1}$$

is readily obtained. It is clear from this relation that g_n is a polynomial in E of degree n . We also know that G is a polynomial function of degree M and so we must have $g_{M+1} = 0$. The $M + 1$ roots of g_{M+1} are precisely the energy levels E_m . Moreover, the eigenstates (4) are expressible as (up to overall normalisation)

$$|v_1, \dots, v_M\rangle = \sum_{n=0}^M g_n (\hat{b}^\dagger)^{(M-n)} (\hat{a}^\dagger \hat{a}^\dagger / 2)^n |\Psi\rangle. \quad (5)$$

We have implemented these results in order to numerically solve the energy spectrum for various ranges of the coupling parameters. The numerical results show that good scaling behaviour holds for the entire range of the couplings, even for small particle numbers. A typical example for the coherence correlator is shown below. We remark that the result for the atomic occupation shown in the inset is in qualitative agreement with Fig. 1 of [23].

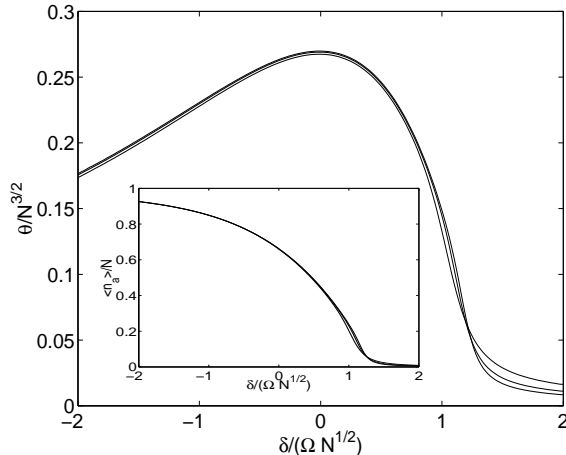


FIG. 1. Scaling behaviour of the coherence correlator for the ground state as a function of the scaled detuning δ . The curves shown are for a total atom number of $N = 20, 30$ and 40 . The threshold coupling for formation of the predominantly molecular BEC state is $\delta/(\Omega\sqrt{N}) \approx 1.4$, indicating that there is a wide range of the scaled detuning δ below threshold for which the ground state consists of a coherent superposition of the atomic and molecular states. The inset shows the average fractional occupation of the atomic state in the ground state.

Some striking features which we have observed are that for fixed N there are no level crossings in the energy spectrum over the entire range of couplings, and the existence of a parity effect for the size of the gap dependent on whether the total atomic number N is odd or even, as illustrated in Fig. 2.

The analysis of Vardi *et al.* [12] in the limit of large N has shown, for an entire population of molecular modes, the existence of two stationary points $|\delta/\Omega| = \sqrt{2N}$, and for $|\delta/\Omega| < \sqrt{2N}$ this state becomes unstable. Our numerical analysis for finite N shows that a similar situation occurs but the gap never vanishes. From Fig. 2 we see that the minimum value for Δ/δ occurs very close to $\delta = \Omega\sqrt{2N}$. For $\delta/\Omega > \sqrt{2N}$ the state consisting entirely of molecules is approximately the ground state which is stable due to the large gap to the next excited level. (The same argument also applies to the negative δ/Ω , which simply follows from the inherent symmetry in the Hamiltonian (1)).

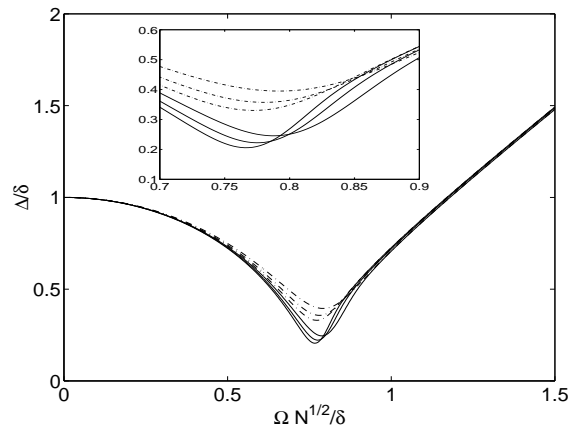


FIG. 2. Reduction in the energy gap to the first excited state near the threshold coupling for formation of the predominantly molecular BEC. In other words, near threshold quantum fluctuations lead to a significant reduction in the binding energy of the molecules. However, note that the energy gap never vanishes for finite N , in contrast to the treatment of Vardi *et al.* [12]. The inset shows a significant parity effect. Near threshold the gap is larger for an odd number of atoms than for an even number of atoms. The solid (dash) curves shown are for $N = 70, 90, 110$ (71, 91, 111).

Quantum dynamics. For an initial state $|\phi(0)\rangle$, the time evolution is given by $|\phi(t)\rangle = U(t)|\phi(0)\rangle$, with $U(t) = \sum_{m=0}^M |m\rangle\langle m| \exp(-iE_m t)$ where $|m\rangle$ is the eigenstate with energy E_m . We also let $g_n(m)$ denote the co-efficients in (5) for $|m\rangle$. Setting $\hat{s} \equiv (2\hat{b}^\dagger\hat{b} - \hat{a}^\dagger\hat{a})/N$, and taking the initial state as the pure molecular state; i.e. $|\phi(0)\rangle = (1/\sqrt{M!})(\hat{b}^\dagger)^M |\psi\rangle$, then we have

$$\begin{aligned} \langle \hat{s}(t) \rangle &= 1 - (4k - 1)/N \\ &\quad - \frac{8}{N} \sum_{m \neq m'} \tilde{g}_0(m) \tilde{g}_0(m') \sin^2(\Delta_{mm'} t/2) \\ &\quad \times \sum_{n=0}^M (n+k) \tilde{g}_n(m) \tilde{g}_n(m'), \end{aligned} \quad (6)$$

with

$$\tilde{g}_n = \frac{2^{-n} g_n \sqrt{(M-n)!(2n+2k-\frac{1}{2})!}}{\sqrt{\sum_{m=0}^M 2^{-2m} (M-m)!(2m+2k-\frac{1}{2})! g_m^2}}$$

and $\Delta_{mm'} = E_m - E_{m'}$. Similarly, if the initial state is a pure atomic state, then

$$\begin{aligned} \langle \hat{s}(t) \rangle &= -1 - \frac{8}{N} \sum_{m \neq m'} \tilde{g}_M(m) \tilde{g}_M(m') \sin^2(\Delta_{mm'} t/2) \\ &\quad \times \sum_{n=0}^M (M-n) \tilde{g}_n(m) \tilde{g}_n(m'). \end{aligned} \quad (7)$$

From the expression for $\langle \hat{s}(t) \rangle$, we see that the short time behavior is quadratic rather than linear in t , due to the square of the sine functions, which is qualitatively consistent with the results of Vardi *et al.* [12] using a linearized model. As for the long time behavior, one can

see that (i) when $N = 2$ and 3 , there are only two levels, so it is always periodic. (ii) when δ/Ω is large and positive, the ground state and first excited state dominate the dynamics, since in this regime, the molecular state is approximately the ground state. As the energy levels are almost equidistant, the evolution is quasi-periodic (with period $T \approx 2\pi/\Delta$) and stable. A similar situation prevails for largely negative δ/Ω . (iii) when δ/Ω is small, all the eigenstates are involved in the evolution due to strong entanglement. This means, all $g_n(m)$ are of the same order for all $|m\rangle$. In this regime, the levels are not uniformly distributed, so $\langle \hat{s}(t) \rangle$ is a non-trivial sum of functions $\sin^2(\Delta_{mm'}t)$ with coefficients depending on $g_n(m)$ and $g_n(m')$. Therefore, the evolution is not quasi-periodic.

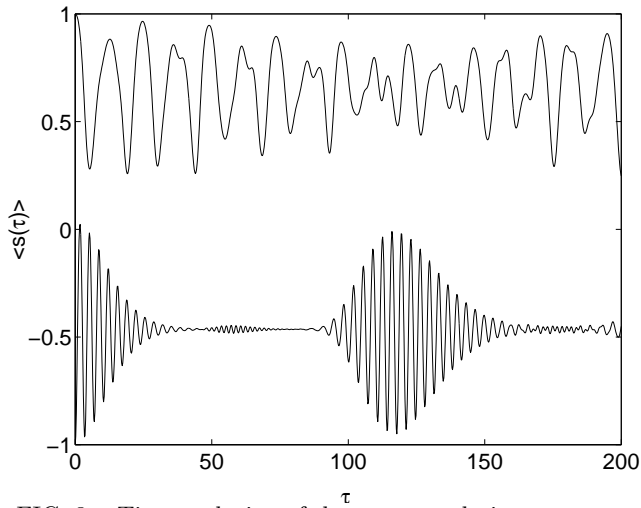


FIG. 3. Time evolution of the average relative atom number $\langle \hat{s}(\tau) \rangle$, where $\tau = \Omega\sqrt{N}t$ is the scaled time. The upper curve depicts evolution of an initial molecular state for $N = 40$ and $|\delta/\Omega| = 6$ (below threshold coupling). Clearly the dynamics are non-periodic. The lower curve shows collapse and revival behaviour for an initial atomic state for the same parameters.

Vardi *et al.* [12] claim that in the large N limit the molecular state is stationary when $\delta/\Omega = \sqrt{2N}$. Observe however that the molecular state is never an eigenstate of the Hamiltonian for finite δ/Ω . Hence for the molecular state to be stationary it is implied that the gap between the ground and first excited state closes. For a large but finite N , the gap does not close (compare Fig. 2). Our conclusion is that there is a smooth transition from the large amplitude, non-periodic coherent oscillations (small δ/Ω) to the quasi-periodic and stable regime (large δ/Ω), supported by Figs. 3 and 4. Our results are in contrast to Fig. 2 in Ref. [12] where the relative population was shown for a sufficiently short time interval that only the collapse was seen and on this basis it was mistakenly suggested that this model can describe decoherence effects.

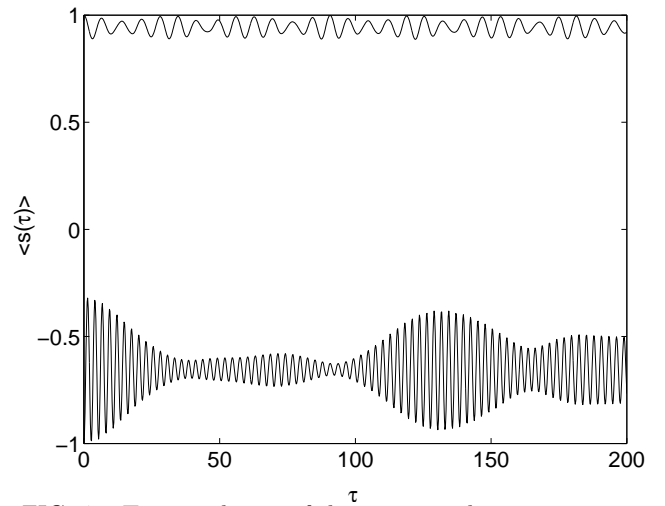


FIG. 4. Time evolution of the average relative atom number for $N=40$ and $|\delta/\Omega| = 10$ (above threshold coupling). The upper curve for an initial molecular state shows stable quasi-periodic behaviour. The lower curve for an initial atomic state illustrates the transition from large amplitude collapse and revival to more stable, small amplitude oscillations, as the detuning δ is increased.

Conclusion. We have shown that a two-mode model for an atom-molecule BEC is exactly solvable via the Bethe ansatz. We have conducted both asymptotic and numerical analysis to establish scaling invariance of the model, identified a parity effect in the energy spectrum and investigated the quantum dynamics. Our results indicate that the transition between the atomic and molecular BEC regimes is smooth, in contrast with Ref. [12]. We believe that the exact solution will help to clarify many facets of the coherence properties of this model, in order to qualitatively compare with current experimental work [5].

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* E-mail: hqz@maths.uq.edu.au

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